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Vibrational spectra and internal rotation of 1,2-diphenylethane

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Abstract

Internal rotation of 1,2-diphenylethane has been studied. Infrared absorption spectra of 1,2-diphenylethane in crystalline phase, liquid and solutions at various temperatures have been investigated. Assignment of the peaks to trans and gauche conformations was performed. Band fitting and factor analysis were applied to conformationally sensitive regions of the spectra. Enthalpy and entropy differences of the conformers were determined and discussed in frames of the reaction field model.

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Keywords

Conformational equilibrium, Infrared spectra, Internal rotation